Usage Report for Fiscal Year 2018

Project Title: Electronic structure calculation on adhesive interface

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1. Background and purpose of the project, relationship of the project with other projects

Adhering substances to each other is one of the technologies directly linked to our lives. The substance is used for adhesion bonds two substances by forming some physical or chemical bonding. However, it is not clear that mechanism at its molecular level. In situ observation by soft X-ray Absorption Spectroscopy (XAS) is conducted to investigate the state of the interface. Model calculation is required to interpret the spectrum. In this research, we construct a structure simulating the adhesive interface to the first principle level. By comparing the experimental and calculated spectrum, we clarify the structure of the adhesive interface and clarify the adhesion mechanism.

2. Specific usage status of the system and calculation method

We got several model structures of adhesive polymer such as TGDDM (tetraglycidyl 4,4'- diamino-diphenylmethane) epoxy resin cured with DDS (4,4'-diaminodiphenylsulfone) from our collaborators of AIST.

The first-principles calculations at the level of DFT level of theory were performed using Gaussian and plane-wave basis sets. XAS calculations were performed using obtained wave functions and its transition moments. Calculations were done with deMon2k 5.0 and Quantum-espresso 5.1.1.

3. Result

Our project has started last month and in this fiscal year I prepared our computational environments and executed several test calculations. We have not obtained computational XAS spectra of our target system yet.

4. Conclusion

In the next fiscal year I will report some research results for computational XAS spectra. To compare experimental results, validity of our models will be examined and elucidation of the mechanism of adhesion interface on molecular level will be aimed.